Table 1. Information on data collection and refinement

Empirical formula: $(C_{47}H_{18}CrF_{15}N_6)\bullet 1.5(C_6H_6)$

Formula weight: 1120.84

Crystallization solvent: benzene/heptane/pyridine

Crystal habit: thin plates

Crystal color: dark violet

Crystal size: 0.40x0.20x0.03 mm^3

Data Collection

Type of diffractometer: Nonius Kappa CCD

Wavelength: 0.71070 Å MoKa

Data collection temperature: 110(2) K

θ range for 7986 reflections used in lattice determination: 2.35 to 25.39°

Unit cell dimension:	a=40.7050(5) Å	α=90.0000(18)°
	b=8.7400(9) Å	β=98.191(2)°
	b=26.9990 Å	γ=90.000(6)°

Volume: 9507.2(12) $Å^3$

Z: 8

Crystal system: monoclinic

Space group: C2/c

Density: 1.566 Mg/m^3

F(000): 4512

θ range for data collection: 2.35 to 25.39°

Index ranges: $0 \leq h \leq 48$, $0 \leq k \leq 8$, $-32 \leq l \leq 31$

Data collection scan type: 0.7 deg. ϕ scans

Reflections collected: 7986

Reflections above threshold [$I > 2\sigma(I)$]: 3845

Absorption coefficient: 0.348 mm^{-1}

Structure Solution and Refinement

Structure solution program: SIR-92

Primary solution method: Direct methods

Secondary solution method: Difference Fourier map

Hydrogen placement: Inferred from neighboring sites

Structure refinement program: SHELXL-97 (Sheldrick, 1997)

Refinement method: Full matrix least squares on F^2

Data / restraints / parameters: 7986 / 0 / 691

Treatment of hydrogen atoms: Some restrained, some unrestrained

Goodness of fit on F^2: 1.025

Final R indices [$I > 2s(I)$]: R=0.0935, wR=0.1564

R indices (all data): R=0.2273, wR=0.2162

Type of weighting scheme used: calculated weighting scheme applied

Weighting scheme used: $1/(\sigma^2(Fo^2)+(0.0458P)^2+87.5606P)$ where

$$P=(Fo^2+2Fc^2)/3$$

Max shift/error: 0.044

Mean shift/error: 0.006

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 2 . Final value of refined atomic coordinates

			Coordinates			Uij					
Num	Label	SFAC									
1	C1	1	0.036	0.144	0.139	0.0280	0.0200	0.0260	0.0010	0.0040	0.0010
2	C2	1	0.019	0.109	0.180	0.0290	0.0520	0.0330	0.0060	0.0130	0.0030
3	C3	1	0.043	0.105	0.222	0.0390	0.0420	0.0210	0.0120	0.0190	0.0070
4	C4	1	0.074	0.142	0.208	0.0390	0.0320	0.0130	-0.0010	0.0110	0.0060
5	C5	1	0.106	0.168	0.235	0.0410	0.0310	0.0140	0.0030	0.0070	0.0050
6	C6	1	0.134	0.225	0.215	0.0350	0.0270	0.0200	0.0000	0.0020	0.0030
7	C7	1	0.168	0.242	0.239	0.0340	0.0560	0.0170	0.0020	-0.0040	0.0100
8	C8	1	0.186	0.292	0.204	0.0270	0.0550	0.0240	-0.0010	-0.0100	0.0040
9	C9	1	0.165	0.307	0.157	0.0270	0.0340	0.0310	-0.0020	0.0020	0.0030
10	C10	1	0.173	0.345	0.109	0.0220	0.0340	0.0290	-0.0020	0.0040	0.0030
11	C11	1	0.152	0.353	0.063	0.0250	0.0350	0.0150	-0.0040	-0.0040	-0.0070
12	C12	1	0.160	0.394	0.015	0.0230	0.0300	0.0320	0.0050	0.0140	0.0000
13	C13	1	0.132	0.392	-0.018	0.0260	0.0310	0.0200	0.0040	0.0050	0.0020
14	C14	1	0.105	0.344	0.008	0.0290	0.0250	0.0220	0.0030	0.0100	-0.0010
15	C15	1	0.071	0.320	-0.010	0.0240	0.0360	0.0170	0.0020	0.0000	0.0060
16	C16	1	0.047	0.259	0.017	0.0270	0.0310	0.0130	-0.0080	0.0020	-0.0040
17	C17	1	0.012	0.241	0.006	0.0260	0.0480	0.0220	0.0040	-0.0040	-0.0020
18	C18	1	0.001	0.187	0.048	0.0240	0.0440	0.0340	0.0010	-0.0030	-0.0090
19	C19	1	0.028	0.175	0.086	0.0320	0.0290	0.0170	-0.0040	0.0070	0.0020
20	C25	1	0.111	0.123	0.289	0.0310	0.0420	0.0140	0.0050	0.0080	0.0070
21	C26	1	0.109	-0.028	0.304	0.0450	0.0440	0.0220	-0.0050	-0.0020	0.0080
22	C27	1	0.115	-0.074	0.353	0.0400	0.0390	0.0220	0.0120	0.0010	-0.0010
23	C28	1	0.122	0.034	0.389	0.0380	0.0580	0.0080	0.0100	0.0040	0.0070
24	C29	1	0.124	0.184	0.377	0.0320	0.0540	0.0170	-0.0100	-0.0010	0.0020
25	C30	1	0.118	0.228	0.328	0.0450	0.0270	0.0270	0.0040	0.0080	0.0090
26	C31	1	0.226	0.502	0.130	0.0470	0.0550	0.0680	0.0270	-0.0190	-0.0150
27	C32	1	0.259	0.527	0.127	0.0300	0.1130	0.1270	0.0330	-0.0220	-0.0250
28	C33	1	0.277	0.436	0.102	0.0230	0.2000	0.1390	0.1230	0.0070	-0.0080
29	C34	1	0.261	0.310	0.078	0.0290	0.1630	0.0890	0.0780	0.0220	0.0330
30	C35	1	0.228	0.283	0.082	0.0400	0.0780	0.0430	0.0380	0.0110	0.0100
31	C36	1	0.209	0.377	0.108	0.0280	0.0460	0.0250	0.0140	-0.0020	0.0070
32	C37	1	0.060	0.370	-0.063	0.0260	0.0290	0.0180	0.0020	0.0060	0.0010
33	C38	1	0.060	0.522	-0.076	0.0270	0.0420	0.0130	-0.0010	-0.0020	-0.0020
34	C39	1	0.049	0.573	-0.124	0.0430	0.0340	0.0230	0.0130	0.0120	0.0070
35	C40	1	0.038	0.471	-0.161	0.0360	0.0610	0.0190	0.0130	0.0020	-0.0040
36	C41	1	0.037	0.319	-0.149	0.0510	0.0530	0.0160	-0.0130	-0.0020	-0.0140
37	C42	1	0.048	0.270	-0.101	0.0370	0.0410	0.0180	-0.0030	0.0030	-0.0040
38	C44	1	0.127	-0.068	0.135	0.0370	0.0360	0.0170	0.0050	0.0020	0.0010
39	C45	1	0.142	-0.205	0.128	0.0420	0.0320	0.0310	0.0070	0.0060	0.0110
40	C46	1	0.143	-0.255	0.080	0.0470	0.0310	0.0350	-0.0010	0.0170	0.0040
41	C47	1	0.128	-0.166	0.041	0.0620	0.0290	0.0270	-0.0020	0.0080	-0.0030

42	C48	1	0.114	-0.028	0.051	0.0400	0.0290	0.0210	-0.0030	0.0030	0.0040
43	C50	1	0.070	0.571	0.092	0.0280	0.0390	0.0220	-0.0020	0.0020	-0.0080
44	C51	1	0.057	0.715	0.101	0.0280	0.0270	0.0410	0.0060	-0.0030	-0.0030
45	C52	1	0.053	0.751	0.149	0.0340	0.0320	0.0520	-0.0050	0.0070	-0.0030
46	C53	1	0.061	0.644	0.186	0.0570	0.0420	0.0390	-0.0060	0.0210	0.0090
47	C54	1	0.075	0.506	0.174	0.0560	0.0370	0.0170	-0.0020	0.0090	0.0050
48	C55	1	0.218	-0.276	-0.019	0.0550	0.0500	0.2800	0.0720	0.0000	0.0150
49	C56	1	0.226	-0.178	0.017	0.1300	0.0730	0.2100	0.0110	0.0980	-0.0050
50	C57	1	0.258	-0.149	0.036	0.1430	0.1150	0.2800	-0.0090	-0.0350	0.0100
51	C58	1	0.315	0.250	0.224	0.1900	0.2600	0.1330	0.1180	0.0750	0.1240
52	C59	1	0.324	0.143	0.190	0.1520	0.1110	0.3000	0.0710	0.1400	0.0390
53	C60	1	0.302	0.035	0.169	0.1190	0.1730	0.2500	0.1460	0.0680	0.0670
54	C61	1	0.270	0.032	0.181	0.0970	0.4100	0.3000	0.2700	0.0470	0.0800
55	C62	1	0.260	0.138	0.214	0.1020	0.7500	0.1300	0.1500	0.0340	0.1800
56	C63	1	0.283	0.247	0.236	0.1800	0.6500	0.0740	0.0500	0.0540	0.2300
57	H2	2	-0.004	0.091	0.179	0.0450	0.0000	0.0000	0.0000	0.0000	0.0000
58	H3	2	0.038	0.081	0.255	0.0390	0.0000	0.0000	0.0000	0.0000	0.0000
59	H7	2	0.175	0.221	0.273	0.0440	0.0000	0.0000	0.0000	0.0000	0.0000
60	H8	2	0.209	0.313	0.210	0.0440	0.0000	0.0000	0.0000	0.0000	0.0000
61	H12	2	0.182	0.418	0.007	0.0330	0.0000	0.0000	0.0000	0.0000	0.0000
62	H13	2	0.130	0.417	-0.052	0.0310	0.0000	0.0000	0.0000	0.0000	0.0000
63	H17	2	-0.001	0.261	-0.026	0.0390	0.0000	0.0000	0.0000	0.0000	0.0000
64	H18	2	-0.022	0.163	0.051	0.0410	0.0000	0.0000	0.0000	0.0000	0.0000
65	H44	2	0.126	-0.036	0.169	0.0360	0.0000	0.0000	0.0000	0.0000	0.0000
66	H45	2	0.152	-0.265	0.156	0.0420	0.0000	0.0000	0.0000	0.0000	0.0000
67	H46	2	0.153	-0.350	0.074	0.0440	0.0000	0.0000	0.0000	0.0000	0.0000
68	H47	2	0.128	-0.199	0.007	0.0470	0.0000	0.0000	0.0000	0.0000	0.0000
69	H48	2	0.104	0.032	0.024	0.0360	0.0000	0.0000	0.0000	0.0000	0.0000
70	H50	2	0.073	0.546	0.058	0.0360	0.0000	0.0000	0.0000	0.0000	0.0000
71	H51	2	0.052	0.786	0.075	0.0390	0.0000	0.0000	0.0000	0.0000	0.0000
72	H52	2	0.044	0.848	0.157	0.0470	0.0000	0.0000	0.0000	0.0000	0.0000
73	H53	2	0.058	0.665	0.220	0.0540	0.0000	0.0000	0.0000	0.0000	0.0000
74	H54	2	0.081	0.436	0.201	0.0430	0.0000	0.0000	0.0000	0.0000	0.0000
75	H55	2	0.195	-0.291	-0.033	0.1550	0.0000	0.0000	0.0000	0.0000	0.0000
76	H56	2	0.209	-0.127	0.031	0.1590	0.0000	0.0000	0.0000	0.0000	0.0000
77	H57	2	0.263	-0.073	0.061	0.2210	0.0000	0.0000	0.0000	0.0000	0.0000
78	H58	2	0.330	0.324	0.238	0.2280	0.0000	0.0000	0.0000	0.0000	0.0000
79	H59	2	0.346	0.145	0.182	0.2140	0.0000	0.0000	0.0000	0.0000	0.0000
80	H60	2	0.308	-0.038	0.146	0.2140	0.0000	0.0000	0.0000	0.0000	0.0000
81	H61	2	0.254	-0.042	0.166	0.3200	0.0000	0.0000	0.0000	0.0000	0.0000
82	H62	2	0.238	0.136	0.223	0.3890	0.0000	0.0000	0.0000	0.0000	0.0000
83	H63	2	0.276	0.319	0.259	0.3540	0.0000	0.0000	0.0000	0.0000	0.0000
84	F1	3	0.103	-0.139	0.269	0.0920	0.0380	0.0240	-0.0040	0.0010	-0.0010
85	F2	3	0.114	-0.223	0.365	0.0710	0.0520	0.0350	0.0150	0.0110	0.0030
86	F3	3	0.128	-0.009	0.438	0.0530	0.0770	0.0180	0.0100	0.0080	0.0150
87	F4	3	0.131	0.291	0.413	0.0690	0.0640	0.0260	-0.0110	0.0060	0.0050
88	F5	3	0.119	0.378	0.317	0.0700	0.0380	0.0270	-0.0070	0.0050	0.0020
89	F6	3	0.210	0.601	0.156	0.0800	0.0530	0.0890	0.0010	-0.0450	-0.0150
90	F7	3	0.274	0.652	0.152	0.0910	0.1250	0.1950	0.0850	-0.0830	-0.0730
91	F8	3	0.309	0.462	0.099	0.0180	0.2780	0.2330	0.1750	0.0100	-0.0170
92	F9	3	0.278	0.215	0.052	0.0670	0.2390	0.1160	0.0820	0.0610	0.0780
93	F10	3	0.214	0.157	0.059	0.0650	0.0880	0.0490	0.0060	0.0220	0.0350
94	F11	3	0.070	0.629	-0.041	0.0380	0.0370	0.0280	-0.0010	-0.0040	-0.0020
95	F12	3	0.050	0.724	-0.135	0.0430	0.0510	0.0390	0.0180	0.0040	0.0030
96	F13	3	0.028	0.519	-0.208	0.0630	0.0890	0.0170	0.0170	-0.0040	0.0000
97	F14	3	0.027	0.214	-0.185	0.0760	0.0790	0.0220	-0.0110	-0.0010	-0.0140
98	F15	3	0.048	0.118	-0.092	0.0720	0.0370	0.0300	-0.0050	0.0020	-0.0100
99	N21	4	0.069	0.162	0.158	0.0250	0.0310	0.0170	0.0030	0.0030	0.0010
100	N22	4	0.133	0.268	0.165	0.0190	0.0330	0.0220	-0.0010	0.0040	-0.0030
101	N23	4	0.119	0.325	0.058	0.0220	0.0260	0.0160	0.0050	-0.0030	-0.0050
102	N24	4	0.056	0.217	0.066	0.0230	0.0280	0.0080	0.0060	0.0000	-0.0010
103	N43	4	0.114	0.026	0.098	0.0340	0.0260	0.0160	-0.0010	0.0060	-0.0070
104	N49	4	0.079	0.467	0.128	0.0240	0.0340	0.0250	0.0010	0.0040	-0.0030
105	Cr	5	0.096	0.246	0.112	0.0280	0.0308	0.0152	0.0007	0.0034	-0.0013

Table 3. Bond distances (Å)

Atom	A	B	Dist
	C1	N21	1.369
	C1	C2	1.425
	C1	C19	1.446

C2	H2	0.949
C2	C3	1.377
C2	C1	1.425
C3	H3	0.952
C3	C2	1.377
C3	C4	1.419
C4	N21	1.364
C4	C3	1.419
C4	C5	1.424
C5	C6	1.410
C5	C4	1.424
C5	C25	1.491
C6	N22	1.398
C6	C5	1.410
C6	C7	1.435
C7	H7	0.951
C7	C8	1.362
C7	C6	1.435
C8	H8	0.950
C8	C7	1.362
C8	C9	1.440
C9	N22	1.370
C9	C10	1.436
C9	C8	1.440
C10	C11	1.403
C10	C9	1.436
C10	C36	1.491
C11	N23	1.367
C11	C10	1.403
C11	C12	1.434
C12	H12	0.949
C12	C13	1.359
C12	C11	1.434
C13	H13	0.950
C13	C12	1.359
C13	C14	1.438
C14	N23	1.391
C14	C15	1.405
C14	C13	1.438
C15	C14	1.405
C15	C16	1.429
C15	C37	1.498
C16	N24	1.365
C16	C17	1.425
C16	C15	1.429
C17	H17	0.951
C17	C18	1.377
C17	C16	1.425
C18	H18	0.952
C18	C17	1.377
C18	C19	1.394
C19	C18	1.394
C19	N24	1.394
C19	C1	1.446

C25	C26	1.388
C25	C30	1.392
C25	C5	1.491
C26	F1	1.349
C26	C27	1.377
C26	C25	1.388
C27	F2	1.344
C27	C28	1.358
C27	C26	1.377
C28	F3	1.352
C28	C29	1.357
C28	C27	1.358
C29	F4	1.355
C29	C28	1.357
C29	C30	1.371
C30	F5	1.343
C30	C29	1.371
C30	C25	1.392
C31	F6	1.348
C31	C36	1.377
C31	C32	1.385
C32	C33	1.318
C32	F7	1.373
C32	C31	1.385
C33	C32	1.318
C33	F8	1.324
C33	C34	1.392
C34	F9	1.341
C34	C35	1.390
C34	C33	1.392
C35	F10	1.352
C35	C36	1.369
C35	C34	1.390
C36	C35	1.369
C36	C31	1.377
C36	C10	1.491
C37	C38	1.377
C37	C42	1.384
C37	C15	1.498
C38	F11	1.356
C38	C39	1.373
C38	C37	1.377
C39	F12	1.354
C39	C40	1.368
C39	C38	1.373
C40	F13	1.344
C40	C41	1.366
C40	C39	1.368
C41	F14	1.358
C41	C40	1.366
C41	C42	1.374
C42	F15	1.352
C42	C41	1.374
C42	C37	1.384

C44	H44	0.950
C44	N43	1.350
C44	C45	1.370
C45	H45	0.950
C45	C44	1.370
C45	C46	1.378
C46	H46	0.949
C46	C47	1.373
C46	C45	1.378
C47	H47	0.950
C47	C46	1.373
C47	C48	1.379
C48	H48	0.949
C48	N43	1.348
C48	C47	1.379
C50	H50	0.950
C50	N49	1.342
C50	C51	1.397
C51	H51	0.950
C51	C52	1.377
C51	C50	1.397
C52	H52	0.949
C52	C53	1.374
C52	C51	1.377
C53	H53	0.951
C53	C52	1.374
C53	C54	1.377
C54	H54	0.951
C54	N49	1.335
C54	C53	1.377
C55	H55	0.948
C55	C56	1.310
C55	C57	1.321
C56	H56	0.950
C56	C55	1.310
C56	C57	1.358
C57	H57	0.951
C57	C55	1.321
C57	C56	1.358
C58	H58	0.951
C58	C63	1.388
C58	C59	1.392
C59	H59	0.950
C59	C60	1.390
C59	C58	1.392
C60	H60	0.951
C60	C61	1.388
C60	C59	1.390
C61	H61	0.951
C61	C60	1.388
C61	C62	1.390
C62	H62	0.950
C62	C61	1.390
C62	C63	1.392

C63	H63	0.951
C63	C58	1.388
C63	C62	1.392
H2	C2	0.949
H3	C3	0.952
H7	C7	0.951
H8	C8	0.950
H12	C12	0.949
H13	C13	0.950
H17	C17	0.951
H18	C18	0.952
H44	C44	0.950
H45	C45	0.950
H46	C46	0.949
H47	C47	0.950
H48	C48	0.949
H50	C50	0.950
H51	C51	0.950
H52	C52	0.949
H53	C53	0.951
H54	C54	0.951
H55	C55	0.948
H56	C56	0.950
H57	C57	0.951
H58	C58	0.951
H59	C59	0.950
H60	C60	0.951
H61	C61	0.951
H62	C62	0.950
H63	C63	0.951
F1	C26	1.349
F2	C27	1.344
F3	C28	1.352
F4	C29	1.355
F5	C30	1.343
F6	C31	1.348
F7	C32	1.373
F8	C33	1.324
F9	C34	1.341
F10	C35	1.352
F11	C38	1.356
F12	C39	1.354
F13	C40	1.344
F14	C41	1.358
F15	C42	1.352
N21	C4	1.364
N21	C1	1.369
N21	Cr	1.929
N22	C9	1.370
N22	C6	1.398
N22	Cr	1.943
N23	C11	1.367
N23	C14	1.391
N23	Cr	1.951

N24	C16	1.365
N24	C19	1.394
N24	Cr	1.926
N43	C48	1.348
N43	C44	1.350
N43	Cr	2.109
N49	C54	1.335
N49	C50	1.342
N49	Cr	2.129
Cr	N24	1.926
Cr	N21	1.929
Cr	N22	1.943
Cr	N23	1.951
Cr	N43	2.109
Cr	N49	2.129

Table 4. Bond angles (°)

Atom	A	B	C	Angle
	N21	C1	C2	107.13
	N21	C1	C19	114.32
	C2	C1	C19	138.42
	H2	C2	C3	126.47
	H2	C2	C1	126.63
	C3	C2	C1	106.90
	H3	C3	C2	125.59
	H3	C3	C4	125.60
	C2	C3	C4	108.81
	N21	C4	C3	106.40
	N21	C4	C5	119.41
	C3	C4	C5	134.07
	C6	C5	C4	126.33
	C6	C5	C25	117.31
	C4	C5	C25	116.28
	N22	C6	C5	124.01
	N22	C6	C7	106.40
	C5	C6	C7	129.43
	H7	C7	C8	125.67
	H7	C7	C6	125.59
	C8	C7	C6	108.74
	H8	C8	C7	126.03
	H8	C8	C9	126.28
	C7	C8	C9	107.69
	N22	C9	C10	123.64
	N22	C9	C8	107.65
	C10	C9	C8	128.56
	C11	C10	C9	127.85
	C11	C10	C36	116.47
	C9	C10	C36	115.67
	N23	C11	C10	123.75
	N23	C11	C12	107.38

C10	C11	C12	128.85
H12	C12	C13	125.94
H12	C12	C11	125.93
C13	C12	C11	108.13
H13	C13	C12	125.78
H13	C13	C14	125.98
C12	C13	C14	108.24
N23	C14	C15	124.89
N23	C14	C13	106.40
C15	C14	C13	128.71
C14	C15	C16	125.57
C14	C15	C37	117.55
C16	C15	C37	116.82
N24	C16	C17	107.79
N24	C16	C15	119.28
C17	C16	C15	132.76
H17	C17	C18	126.44
H17	C17	C16	126.35
C18	C17	C16	107.21
H18	C18	C17	125.68
H18	C18	C19	125.73
C17	C18	C19	108.59
C18	C19	N24	107.57
C18	C19	C1	141.52
N24	C19	C1	110.67
C26	C25	C30	115.20
C26	C25	C5	121.95
C30	C25	C5	122.82
F1	C26	C27	117.48
F1	C26	C25	119.25
C27	C26	C25	123.23
F2	C27	C28	120.87
F2	C27	C26	120.48
C28	C27	C26	118.65
F3	C28	C29	119.80
F3	C28	C27	119.37
C29	C28	C27	120.80
F4	C29	C28	120.42
F4	C29	C30	119.60
C28	C29	C30	119.96
F5	C30	C29	118.27
F5	C30	C25	119.57
C29	C30	C25	122.13
F6	C31	C36	119.57
F6	C31	C32	118.67
C36	C31	C32	121.75
C33	C32	F7	119.60
C33	C32	C31	122.83
F7	C32	C31	117.57
C32	C33	F8	122.36
C32	C33	C34	117.63
F8	C33	C34	120.01
F9	C34	C35	121.01
F9	C34	C33	119.54

C35	C34	C33	119.44
F10	C35	C36	119.86
F10	C35	C34	116.93
C36	C35	C34	123.21
C35	C36	C31	115.10
C35	C36	C10	121.05
C31	C36	C10	123.80
C38	C37	C42	115.39
C38	C37	C15	120.63
C42	C37	C15	123.97
F11	C38	C39	116.74
F11	C38	C37	120.21
C39	C38	C37	123.05
F12	C39	C40	119.40
F12	C39	C38	120.85
C40	C39	C38	119.73
F13	C40	C41	120.18
F13	C40	C39	120.64
C41	C40	C39	119.17
F14	C41	C40	120.44
F14	C41	C42	119.38
C40	C41	C42	120.08
F15	C42	C41	118.36
F15	C42	C37	119.08
C41	C42	C37	122.54
H44	C44	N43	117.98
H44	C44	C45	117.92
N43	C44	C45	124.10
H45	C45	C44	120.58
H45	C45	C46	120.67
C44	C45	C46	118.75
H46	C46	C47	120.74
H46	C46	C45	120.83
C47	C46	C45	118.43
H47	C47	C46	120.22
H47	C47	C48	120.10
C46	C47	C48	119.68
H48	C48	N43	118.50
H48	C48	C47	118.61
N43	C48	C47	122.89
H50	C50	N49	118.50
H50	C50	C51	118.60
N49	C50	C51	122.90
H51	C51	C52	120.56
H51	C51	C50	120.56
C52	C51	C50	118.88
H52	C52	C53	120.91
H52	C52	C51	120.96
C53	C52	C51	118.13
H53	C53	C52	120.07
H53	C53	C54	120.14
C52	C53	C54	119.79
H54	C54	N49	118.46
H54	C54	C53	118.31

N49	C54	C53	123.23
H55	C55	C56	120.98
H55	C55	C57	121.45
C56	C55	C57	117.57
H56	C56	C55	119.11
H56	C56	C57	119.26
C55	C56	C57	121.63
H57	C57	C55	119.66
H57	C57	C56	119.59
C55	C57	C56	120.74
H58	C58	C63	120.22
H58	C58	C59	119.75
C63	C58	C59	120.04
H59	C59	C60	120.02
H59	C59	C58	120.09
C60	C59	C58	119.89
H60	C60	C61	120.05
H60	C60	C59	119.87
C61	C60	C59	120.08
H61	C61	C60	120.22
H61	C61	C62	119.74
C60	C61	C62	120.05
H62	C62	C61	120.14
H62	C62	C63	119.90
C61	C62	C63	119.96
H63	C63	C58	120.05
H63	C63	C62	119.95
C58	C63	C62	119.99
C4	N21	C1	110.72
C4	N21	Cr	132.06
C1	N21	Cr	116.01
C9	N22	C6	109.52
C9	N22	Cr	123.41
C6	N22	Cr	126.48
C11	N23	C14	109.79
C11	N23	Cr	123.66
C14	N23	Cr	126.20
C16	N24	C19	108.81
C16	N24	Cr	132.42
C19	N24	Cr	117.20
C48	N43	C44	116.01
C48	N43	Cr	122.19
C44	N43	Cr	121.77
C54	N49	C50	117.03
C54	N49	Cr	120.90
C50	N49	Cr	122.00
N24	Cr	N21	80.95
N24	Cr	N22	172.19
N24	Cr	N23	90.85
N24	Cr	N43	92.81
N24	Cr	N49	88.33
N21	Cr	N22	91.30
N21	Cr	N23	171.78
N21	Cr	N43	91.08

N21	Cr	N49	88.39
N22	Cr	N23	96.91
N22	Cr	N43	88.29
N22	Cr	N49	90.48
N23	Cr	N43	88.59
N23	Cr	N49	92.11
N43	Cr	N49	178.65